(idw)

Press release

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05/19/2011

http://idw-online.de/en/news423886

Transfer of Science or Research
Biology, Information technology, Medicine
transregional, national

New software for the interactive visual analysis of protein structure and function

Proteins are essential molecules that participate in most cellular processes. Biologists are therefore particularly interested in the complex relationships between protein structure and function. A key research issue is the study of individual residues, the building blocks of proteins, and their interactions in the 3D protein structure. Scientists at the Max Planck Institute for Informatics, Saarbruecken, Germany, developed innovative software for the detailed analysis and visualization of residue interactions in protein structures.

To date, the 3D structures of several 10,000 proteins have been determined experimentally. The structures are usually visualized and analyzed in 3D viewers to understand protein function on the molecular level. However, the visual complexity of protein structures renders it difficult to focus on individual residues and their long-range molecular interactions.

Researchers at the Max Planck Institute for Informatics now offer the new software tools RINalyzer and RINerator (www.rinalyzer.de) that support the automated generation, visualization, and interactive analysis of residue interaction networks (RINs). A RIN is derived from the corresponding 3D protein structure and consists of network nodes and connecting edge lines that represent protein residues and their interactions, respectively. Recent studies have shown that RINs are especially useful for identifying functionally important residues and characterizing their impact on protein structure and function.

"We already applied RINs successfully to characterize the functional effect of residue changes that are located far away from the drug-binding site in protein structures. In the past, we had to perform the analysis and the visualization manually because no such tool as RINalyzer was available," explains Francisco S. Domingues, who has recently moved from the Max Planck Institute to EURAC research in Bolzano, Italy.

RINalyzer is the first tool that combines the 3D structure view of a protein with its network representation. Protein residues selected in a RIN are automatically highlighted in the 3D protein structure, and vice versa. "To investigate complex protein-structure relationships, we provide molecular biologists with free, user-friendly software. The rich versatility of RINalyzer does not require previous network analysis expertise or programming knowledge from the users," says Nadezhda T. Doncheva, research scientist at the Max Planck Institute.

RINalyzer is complemented by the large online database RINdata that contains over 50,000 precomputed RINs for most protein structures in the publicly available Protein Data Bank. "Our novel tools have the great potential to become a standard application for biologists alongside other existing approaches to protein structure visualization," notes Mario Albrecht, research group leader at the Max Planck Institute in the local Cluster of Excellence on Multimodal Computing and Interaction.

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